



```

chain nodes :
  7 8 9 19 20 27 28 42 43 44 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73
  74 75 76 80 83 90 97 98
ring nodes :
  1 2 3 4 5 6 10 11 12 13 14 15 16 17 18 21 22 23 24 25 26 29 30 31 32
  33 34 35 36 37 38 39 40 41 45 46 47 48 49 50 51 52 53 54 55 56 57 58 82
chain bonds :
  3-9 4-8 6-7 16-20 18-19 24-28 26-27 30-43 31-42 32-97 41-44 43-62 46-60 47-59
  48-80 49-98 58-61 60-73 62-63 64-65 65-66 66-67 66-90 70-71 75-76 82-83
ring bonds :
  1-6 1-2 2-3 3-4 4-5 5-6 10-11 10-12 11-13 12-14 13-14 13-15 14-18 15-16 16-17
  17-18 21-26 21-22 22-23 23-24 24-25 25-26 29-30 29-32 30-31 31-82 32-82 33-34
  33-35 34-36 35-37 36-37 36-38 37-41 38-39 39-40 40-41 45-46 45-49 46-47 47-48
  48-49 50-51 50-52 51-53 52-54 53-54 53-55 54-58 55-56 56-57 57-58
exact/norm bonds :
  1-6 1-2 2-3 3-4 4-5 4-8 5-6 6-7 10-11 10-12 11-13 12-14 13-14 13-15 14-18 15-16
  16-17 16-20 17-18 18-19 21-26 21-22 22-23 23-24 24-25 25-26 29-30 29-32 30-31 31-82 32-97
  29-32 30-31 31-42 31-82 32-97 32-82 33-34 33-35 34-36 35-37 41-44 45-46 45-49
  46-47 47-48 47-59 48-49 48-80 49-98 50-51 50-52 51-53 52-54 58-61 62-63 62-64
  64-65 65-66 66-67 66-90 82-83
exact bonds :
  3-9 30-43 43-62 46-60 60-73 70-71 75-76
normalized bonds :
  36-37 36-38 37-41 38-39 39-40 40-41 53-54 53-55 54-58 55-56 56-57 57-58

```

G1:[*1],[*2]

G2:[*3],[*4],[*5],[*6],[*7]

G3:[*8],[*9],[*10],[*11],[*12]

Match level :

```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS 20:CLASS 21:Atom
22:Atom

```

23:Atom 24:Atom 25:Atom 26:Atom 27:CLASS 28:CLASS 29:Atom 30:Atom 31:Atom
32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom
42:CLASS 43:CLASS 44:CLASS 45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom
52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 57:Atom 58:Atom 59:CLASS 60:CLASS 61:CLASS
62:CLASS 63:CLASS 64:CLASS 65:CLASS 66:CLASS 67:CLASS 68:CLASS 69:CLASS 70:CLASS
71:CLASS 72:CLASS 73:CLASS 74:CLASS 75:CLASS 76:CLASS 80:Atom 82:Atom 83:Atom 90:CLASS
97:CLASS 98:CLASS